NON-COMMUTATIVE BLOCH THEORY: AN OVERVIEW

Michael J. Gruber

Institute of Mathematics, Humboldt University at Berlin, Germany

E-mail: gruber@mathematik.hu-berlin.de

WWW: http://spectrum.mathematik.hu-berlin.de/~gruber

Abstract

For differential operators which are invariant under the action of an abelian group Bloch theory is the tool of choice to analyze spectral properties. By shedding some new non-commutative light on this we motivate the introduction of a non-commutative Bloch theory for elliptic operators on Hilbert C*-modules. It relates properties of C*-algebras to spectral properties of module operators such as band structure, weak genericity of cantor spectra, and absence of discrete spectrum. It applies e.g. to differential operators invariant under a projective group action, such as Schrödinger operators with periodic magnetic field.

INTRODUCTION

Bloch (or Floquet) theory in its usual form already has a long history. Basically it starts from the fact that partial differential equations with constant coefficients are mapped into algebraic equations by means of the Fourier or Laplace transform. Now, if the coefficients are not constant but just periodic under an abelian (locally compact topological) group one still has the Fourier transform on such groups, mapping functions on the group Γ into functions on the dual group $\hat{\Gamma}$; the original spectral problem on a non-compact manifold is mapped into a (continuous) sum of spectral problems on a compact manifold (see section 1).

This is what makes Bloch theory an indispensible tool especially for solid state physics, where one describes the motion of non-interacting electrons in a periodic solid crystal by a Schrödinger operator $-\Delta + V$ on $L^2(\mathbb{R}^d)$. The potential function V is the gross electric potential generated by all the crystal ions and thus is periodic under the lattice given by the crystal symmetry.

Measurements of crystals often require magnetic fields b (2-form). In quantum mechanics, they are described by a vector potential (1-form) a such that b = da (B = da)

 $\operatorname{curl} A$ for the corresponding vector fields). The magnetic Schrödinger operator then reads

$$H = -(\nabla - ia)^2 + V.$$

But, although b is periodic or even constant, a need not be so, and H won't be periodic. It is therefore necessary to use magnetic translations (first introduced by Zak [2]) under which H still is invariant. But now, these translations do not commute with each other in general. Therefore ordinary (commutative) Bloch theory does not apply.

Basically, the reason for this failure is that a non-abelian group has no "good" group dual: the set of (equivalence classes of) irreducible representations has no natural group structure whereas the set of one-dimensional representations is too small to describe the group — otherwise it would be abelian.

But although $\hat{\Gamma}$ does not exist any more, the algebra $C(\hat{\Gamma})$ of continuous functions continues to exist in some sense: It is given by the reduced group C*-algebra of Γ which is just the C*-algebra generated by Γ in its regular representation on itself (on $l^2(\Gamma)$).

Section 2 shows how one can re-formulate ordinary Bloch theory in a way which refrains from using the points of $\hat{\Gamma}$ and relies just on the rôle of $C(\hat{\Gamma})$. From a technical point of view this requires switching from measurable fields of Hilbert spaces to continuous fields which then can be described as Hilbert C*-modules over the commutative C*-algebra $C(\hat{\Gamma})$.

Having done this one can retain the setup but omit the condition of commutativity for the C*-algebra $C(\hat{\Gamma})$. Thus one is lead to non-commutative Bloch theory (section 3) dealing with elliptic operators on Hilbert C*-modules over non-commutative C*-algebras. The basic task is now to relate properties of the C*-algebra to spectral properties of "periodic" operators. Thus one generalizes spectral results for elliptic operators on compact manifolds as well as results of ordinary Bloch theory.

In section 4 we list examples where non-commutative Bloch theory applies.

This article is an overview of a part of my Ph.D. thesis [10] which is written in German. Due to space limitations the following sections will be rather sketchy. A full account of that part in English is in preparation [13], as well as for the other, related parts [11, 12]. I am indepted to my thesis advisor Jochen Brüning for scientific support.

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1. COMMUTATIVE BLOCH THEORY

Setup

Let X be a smooth oriented Riemannian manifold and Γ a discrete abelian group, acting on X properly discontinuously ($\Rightarrow M := X/\Gamma$ is Hausdorff), freely ($\Rightarrow M$ smooth),

isometrically ($\Rightarrow M$ Riemannian), and co-compactly ($\Leftrightarrow M$ compact). The Γ -action on X induces an action on $C_{(c)}^{\infty}(X)$ and a unitary action on $L^2(X)$ via

$$(\gamma_* f)(x) := f(\gamma^{-1} x)$$

for $x \in X, \gamma \in \Gamma$ and f in the corresponding space of functions.

Let D be a symmetric Γ -periodic elliptic differential operator on X, i.e. on its domain of definition $C_c^{\infty}(X) \subset L^2(X)$. By Γ -periodic we mean that D commutes with the Γ -action on its domain.

The basic physical example is $X = \mathbb{R}^d$ (d = 2,3), $\Gamma = \mathbb{Z}^d$ acting by translations (or magnetic translations) and D given by the Schrödinger operator (or magnetic Schrödinger operator with integral flux) with periodic electric potential.

Aim

Our aim is to determine the type (set/measure theoretic) of the spectrum of D. By set theoretic type of the spectrum¹ we mean either **band structure** (i.e. a locally finite union of closed intervals) or **Cantor structure** (i.e. a nowhere dense set without isolated points). Bands may degenerate to points which would not be called bands by physicists. Non-degenerate bands allow formation of (semi-) conductors.

Measure theoretic properties of the spectrum are continuity properties of the spectral measure with respect to Lebesgue measure. Physically one expects either pure point spectrum (eigenvalues and their accumulation points) or absolutely continuous spectrum (bands). Thus one wants to exclude the third possibility: singular continuous spectrum.

Method

The basic and well-known method for the spectral theory of periodic elliptic operators is **Bloch theory**, which in one dimension is also called **Floquet theory**. Its first step is to construct a direct integral

$$L^2(X) \simeq \int_{\hat{\Gamma}}^{\oplus} H_{\chi} \, d\chi,$$
 (1.1)

$$D \simeq \int_{\hat{\Gamma}}^{\oplus} D_{\chi} \, d\chi,\tag{1.2}$$

where the fiber Hilbert spaces

$$H_{\gamma} = L^2(F_{\gamma}) \tag{1.3}$$

¹Under the aforementioned conditions D is essentially self-adjoint, so that the closure of D is the only self-adjoint extension and has only real spectrum. By abuse of notation we denote the closure by D, too.

are spaces of square-integrable sections of associated complex line bundles

$$F_{\chi} = X \times_{\chi} \mathbb{C},\tag{1.4}$$

and the operators in the fiber are given by the gauge-periodic boundary conditions

$$D_{\chi} = D|_{C^{\infty}(F_{\chi})}. \tag{1.5}$$

The decomposition $\Phi: L^2(X) \to \int_{\hat{\Gamma}}^{\oplus} H_{\chi} d\chi$ is defined by

$$(\Phi f)(x)_{\chi} := \sum_{\gamma \in \Gamma} \chi(\gamma) f(\gamma^{-1} x) \tag{1.6}$$

for $f \in C_c^{\infty}(X), \chi \in \hat{\Gamma}, x \in X$ and can be extended unitarily to $L^2(X)$.

 $\hat{\Gamma}$ may be identified with the Brillouin zone in solid state physics, H_{χ} is the space of wave functions with quasi-momentum χ . The family $(H_{\chi})_{\chi \in \hat{\Gamma}}$ is a measurable field of Hilbert spaces; decomposability of D w.r.t. this field is equivalent to Γ -periodicity of D.

The decomposition described above is still valid for the magnetic Schrödinger operator with zero magnetic flux per lattice cell but has to be modified for non-zero integral flux. In any case, the fibers D_{χ} may be identified with magnetic Schrödinger operators on the quotient space $M = X/\Gamma$ on which there may be inequivalent quantizations of the classical magnetic system. Indeed, the family $(D_{\chi})_{\chi \in \hat{\Gamma}}$ contains all possible quantization classes ([8, 11]).

Results

By general results for direct integrals (see e.g. [1], chapter II, §1) one can compute the spectrum of D from the spectra of the family $(D_{\chi})_{\chi \in \hat{\Gamma}}$. Using special properties of this family one gets:

- 1. Since $(D_{\chi})_{\chi \in \hat{\Gamma}}$ is a continuous family of operators with compact resolvent, the spectrum of D is given as the union spec $D = \bigcup_{\chi \in \hat{\Gamma}} \operatorname{spec} D_{\chi}$ and thus has band structure. Bands may degenerate to points, but possible eigenvalues have infinite multiplicity automatically.
- 2. Using the real analyticity of the operator family one gets:
 - $\operatorname{spec}_{s.c.} D = \emptyset$
 - $\operatorname{spec}_{p.p.} D$ is discrete as a subset of \mathbb{R} .

For the magnetic Schrödinger operator with zero magnetic flux this is due to [9]; for rational flux (and general abelian-periodic elliptic operators) this was done in [10, 12].

2. COMMUTATIVE BLOCH-THEORY FROM A NON-COMMUTATIVE POINT OF VIEW

As seen above it is necessary to use, in addition to a measurable field of Hilbert spaces, the continuity property of an operator family. Thus the basic idea is to incorporate the continuity into the setup, i.e. to find a continuous sub-field. Now, a continuous field of Hilbert spaces over a space $\hat{\Gamma}$ is equivalent to a Hilbert C*-module over $C(\hat{\Gamma})$. In our geometric context such a module is given naturally: For $e, f \in C_c^{\infty}(X)$ define

$$\langle e|f\rangle_{\mathcal{E}}(\chi) := \langle \Phi(e)_{\chi}|\Phi(f)_{\chi}\rangle_{H_{\chi}}.$$
 (2.1)

This gives a $C(\hat{\Gamma})$ -linear pre-scalar product, completion gives a Hilbert $C(\hat{\Gamma})$ -module \mathcal{E} , periodic operators are adjointable module operators.

How to get back $L^2(X)$ from \mathcal{E} ? This can be done by means of the Hilbert GNS representation: Haar measure $d\chi$ on $\hat{\Gamma}$ defines a faithful state τ on $C(\hat{\Gamma})$ via integration and

$$\langle e|f\rangle_{\tau} = \int_{\hat{\Gamma}} \langle \Phi(e)_{\chi} | \Phi(f)_{\chi} \rangle_{H_{\chi}} = \langle e|f\rangle_{L^{2}(X)}$$
 (2.2)

so that the representation space \mathcal{E}_{τ} is just $L^{2}(X)$.

The second basic observation is that $C(\hat{\Gamma}) = C^*_{red}(\Gamma)$ is the reduced group C*-algebra of Γ , i.e. the C*-algebra generated by Γ in its regular representation on $l^2(\Gamma)$. This algebra continues to exist for non-abelian groups, but will be non-commutative.

3. NON-COMMUTATIVE BLOCH THEORY

Setup

Let \mathcal{A} be a C*-algebra and H a Hilbert space which is a right \mathcal{A} -module. Let D be a (possibly unbounded) self-adjoint operator on H, commuting with the module action of \mathcal{A} . For physical examples we refer to section 4.

Aim

We now want to investigate the relations between spec D and A; in particular this should reproduce the band structure results in the commutative case as described above.

Method

The basic step is to construct a Hilbert \mathcal{A} -module \mathcal{E} and a faithful (tracial) state τ on \mathcal{A} such that the Hilbert GNS representation gives back the Hilbert space on which to do spectral theory: $H \simeq \mathcal{E}_{\tau}$; and such that D comes from an unbounded self-adjoint module operator F on \mathcal{E} which is \mathcal{A} -elliptic (see below). This construction has to be done for each class of examples separately and may require hard analytic work; once they fit into the general framework it is just (\mathbb{C}^* -) algebraic propeties which are used.

Under these assumptions one can construct a trace tr_{τ} on the τ -trace class $\mathcal{L}^1_{\mathcal{A}}(\mathcal{E},\operatorname{tr}_{\tau})$ in the module operators which generalizes the trace per unit volume in solid state physics. Applying this trace to projections one gets as usual a generalized dimension \dim_{τ} for the range of projections.

Ellipticity

Let T be an unbounded operator on \mathcal{E} . T is called \mathcal{A} -elliptic if

- 1. T is densely defined,
- 2. T is regular, i.e. T^* exists, is densely defined, and $\operatorname{ran}(1+T^*T)$ is dense in \mathcal{E} , and
- 3. T has \mathcal{A} -compact resolvent, i.e. $(1+T^*T)^{-1} \in \mathcal{K}_{\mathcal{A}}(\mathcal{E})$.

This is the notion of ellipticity which is usual for operators on Hilbert modules.

Basic criteria

Let \mathcal{C} be a C*-algebra, τ a trace. \mathcal{C} has the **Kadison property** if there is c > 0 such that for all non-zero projections P in \mathcal{C} one has $\tau(P) \geq c$.

Let \mathcal{C} be a C*-algebra, τ a state. \mathcal{C} has **real rank zero with inifinitesimal state** if every self-adjoint element can be approximated by a finite spectrum element with arbitrary small τ -value on the spectral projections.

Results

- 1. If λ is an isolated eigenvalue of D then the corresponding eigenspace H_{λ} is an (algebraically) finitely generated projective Hilbert \mathcal{A} -module. If e^{-D^2} is of τ -trace class then H_{λ} has finite τ -dimension: $\dim_{\tau} H_{\lambda} < \infty$ If \mathcal{E}, \mathcal{A} are "suitable" then H_{λ} is infinite dimensional ($\dim H_{\lambda} = \infty$), in particular the discrete spectrum is empty: spec_{disc} $D = \emptyset$
- 2. If $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ has the Kadison property and e^{-D^2} is of τ -trace class then D has band spectrum (the basic idea going back to [4, 5, 6]).
- 3. If $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ has real rank zero with infinitesimal state (RRI_0) then Cantor spectrum is weakly generic ([3]), i.e. every operator can be approximated by ones with Cantor spectrum in norm resolvent sense.

The first part is analogous to the case of elliptic operators on compact manifolds: these have compact resolvent and therefore finite-dimensional eigenspaces, whereas in our situation we have \mathcal{A} -compact resolvent and finitely generated modules, but (under suitable conditions) infinite-dimensional eigenspaces.

The second part traces back band structure to a property that holds in the commutative case.

The third part gives a citerion for weakly generic (i.e. for a dense set of operators) total break-down of band structure.

4. EXAMPLES

Commutative Bloch theory

 \mathcal{A} is the algebra of continuous functions $C(\hat{\Gamma})$ on the character group, \mathcal{E} the space of sections of a continuous field of Hilbert spaces defined by the continuous Bloch sections. The state τ is given by integration w.r.t. Haar measure: $\tau(f) = \int_{\hat{\Gamma}} f(\chi) d\chi$. From this it follows that $C(\hat{\Gamma})$ has the Kadison property which implies band structure. Furthermore, we are in the "suitable" situation so that any possible eigenspace is infinite-dimensional but has finite τ -dimension.

Periodic elliptic operators

Here \mathcal{A} is the reduced group C*-algebra $C^*_{red}(\Gamma)$ of Γ , \mathcal{E} is defined by

$$\langle e|f\rangle_{\mathcal{E}} := \sum_{\gamma \in \Gamma} \langle T_{\gamma}e|f\rangle_{L^{2}(E)} L_{\gamma}$$

for a vector bundle E over X with lift T_{γ} of the Γ -action; τ is the canonical trace, L_{γ} the left regular representation of Γ on $l^2(\Gamma)$. This reproduces [4, 5].

Gauge-periodic elliptic operators

This case is as above, but additionally with a projective lift U_{γ} of the action such that

$$U_{\gamma_1}U_{\gamma_2} = \Theta(\gamma_1, \gamma_2)U_{\gamma_1\gamma_2}.$$

Therefore Θ defines a group cohomology class $[\Theta] \in H^2(\Gamma, S^1)$, and $\mathcal{A} = C^*_{red}(\Gamma, \Theta)$ is a twisted reduced group C*-algebra, $\mathcal{E} \simeq \mathcal{A} \otimes h$ as above. In particular \mathcal{A} is a rotation algebra \mathcal{A}_{α} for the \mathbb{Z}^2 -periodic magnetic Schrödinger operator, where α denotes the magnetic flux.

If $\alpha \in \mathbb{Q}$ then \mathcal{A} has the Kadison property so that $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ has the Kadison property, too, and D has band spectrum (reproducing [6]).

If $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ then \mathcal{A} has RRI_0 so that $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ has RRI_0 , too, ([7]) and Cantor spectrum is weakly generic.

Hofstadter model, quantum pendulum

This is the case of the difference equations known as almost Matthieu, Hofstadter type or quantum pendulum, arising in several models in solid state physics (Peierls substitution, mesoscopic systems) as well as in integrable systems. Here we have just a trivial Hilbert module $\mathcal{A} = \mathcal{E} = \mathcal{A}_{\alpha}$ over a rotation algebra. Therefore, the results are as above.

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